JOURNAL OF MOLECULAR STRUCTURE, VOLUME 223 (1990)

AUTHOR INDEX

Alonso, J.L., 365
Arai, T., 355

Bauer, S.H., 375
Beaudet, R.A., 15
Borchardt, D.B., 375
Brahms, J.C., 217
Brletic, P.A., 291
Burden, F.R., 345
Bürger, H., 457

Caminati, W., 415
Carrick, P., 171
Charland, J.-P., 115
Cho, H.-G., 231
Cox, A.P., 185
Cradock, S., 457
Craig, N.C., 45
Curl, R.F., 171

Dailey, W.P., 217
Dawes, M., 171
Degli Esposti, A., 325
Di Bernardo, S., 415
Diguiseppe, T., 273
Durig, J.R., 291, 457, 471

Eujen, R., 457

Friedrich, V., 253
Fu-Tai Tuan, D., 123
Fukushima, K., 337

Gillies, C.W., 273
Gillies, J.Z., 273
Golden, S., 93
Goldstone, J.A., 383
González, E., 365
Groner, P., 471

Harada, I., 355
Harmony, M.D., 217
Hayashi, M., 207
Hedgecock, I., 33
Hirota, E., 149

Ikeda, C., 207

Jaworski, A., 63
Judson, R.S., 425
Justnes, H., 273

Kanters, J.A., 287
Kim, H., 45
Kivelson, D., 253
Koester, E., 171
Kooijman, H., 287
Kroon, J., 287
Krusic, P.J., 115
Kubulat, K., 63
Kuczkowski, R.L., 45
Kwei, G.H., 383

Larsen, N.W., 33
Lawson II, A.C., 383
Lehmann, K.K., 425
Li, Y.S., 15, 291
Lister, D.G., 325
Little, T.S., 291
Loar, G.W., 123
López, J.C., 365
Lorenčak, P., 45
Lovas, F.J., 273

Morton, J.R., 115
Murray, K.K., 171

Nygaard, L., 33

Oe, S., 337

Palmieri, P., 325
Pedersen, T., 33
Person, W.B., 63
Petri, M., 171
Preston, K.F., 115

Rabitz, H., 425
Rego, C.A., 185
Reinhardt, W.P., 157
Richnow, M.L., 171
Rickus, L., 273
Ridgen, J.S., 1

Sage, M.L., 407
Saito, K., 375
Scherrenberg, R.L., 287
Schwendeman, R.H., 231
Sibley, S.P., 45
Sørensen, G.O., 33
Stevens, R., 185
Suenram, R.D., 273
Sullivan, J.F., 457
Szczepaniak, K., 63
Szczesniak, M., 63

Takeuchi, H., 355
Tam, H.S., 217
Tarjus, G., 253
Tolley, C.L., 471
Trombetti, A., 415

Von Dreele, R.B., 383

Wang, A.-Y., 291
Wang, E.C., 15
Warburton, W.K., 383
Warren, W.S., 425
Whang, C.M., 457
Williams, A., 383

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 223 (1990)

SUBJECT INDEX

Adiabatic switching,
Calculation of the vib-rotational state density of polyatomic molecules by adiabatic switching, 157
Amino hydrogen location,
Microwave spectrum and amino hydrogen location in 7-azaindole, 415
Anomalous X-ray,
Structure and valence from complementary anomalous X-ray and neutron powder diffraction, 383
Azaindole,
Microwave spectrum and amino hydrogen location in 7-azaindole, 415

Bipyridines,
Raman spectroscopic study of characteristic conformations of bipyridines adsorbed on active electrode surface, 337
Bright Wilson, Jr.,
Quantum mechanics, chemical physics and E. Bright Wilson, Jr., 1
Bromocytosine,
Infrared spectra and tautomerism of 5-fluorocytosine, 5-bromocytosine and 5-iodocytosine. Matrix isolation and theoretical ab initio studies, 63
β-Butyrolactone,
Internal rotation and structure of β-butyrolactone: microwave and ab initio studies, 365

CD_3Br
Infrared-radiofrequency double-resonance spectroscopy of CD_3Br, 231
Cancellation effect,
Local symmetry, multi-body correlations and the cancellation effect, 253
Computer algebra,
Applications of computer algebra to molecular spectroscopy, 407

Deuterated isotopomers,
Conformation of furfurylamine studied by microwave spectra of five deuterated isotopomers of furfurylamine, 33
Dicyclohexano-18-crown-6,
Raman spectra and conformations of dibenzo- and dicyclohexano-18-crown-6, 355
Difluoromethylphosphine,
Microwave spectrum, electric dipole moment and barriers to internal rotation of *trans* and *gauche*-difluoromethyl-phosphine CHF_2PH_2, 15
Difluoropropadienone,
Microwave spectrum, structure and dipole moment of difluoropropadienone, 217
Dynamical molecular structure,
Dynamical molecular structure studied by high resolution spectroscopy, 149

Ethylene carbonate,
A two-dimensional ring puckering potential energy surface for ethylene carbonate from ab initio and flexible model computations, 325
External fields,
Optimal design of external fields for controlling molecular motion: application to rotation, 425

$Fe_3(CO)_{11}^-$ ions,
EPR spectra of $Fe_3(CO)_{11}^-$ ions and $[Fe_3(CO)_{11}^-]_2$ triplet ion-pairs trapped in single crystals of $PPN^+HFe_3(CO)_{11}^-$, 115
Fluorocytosine,
Infrared spectra and tautomerism of 5-fluorocytosine, 5-bromocytosine and 5-iodocytosine. Matrix isolation and theoretical ab initio studies, 63
Furfurylamine,
Conformation of furfurylamine studied by

microwave spectra of five deuterated isotopomers of furfurylamine, 33

Infrared-radiofrequency double resonance spectroscopy,
Infrared-radiofrequency double-resonance spectroscopy of CD_3Br, 231
Iodocytosine,
Infrared spectra and tautomerism of 5-fluorocytosine, 5-bromocytosine and 5-iodocytosine. Matrix isolation and theoretical ab initio studies, 63

Lewis acid/base systems,
Relaxation kinetics in gaseous Lewis acid/base systems: the prototype, $(CH_3)_2O^+BF_3$ $(CH_3)_2O{:}BF_3$, 375
Local symmetry,
Local symmetry, multi-body correlations and the cancellation effect, 253

Methacryloyl chloride,
Rotational and vibrational spectra, conformational stability, potential functions and ab initio calculations of methacryloyl chloride, 291
Methanol,
The OH stretching fundamental of methanol, 171
Methoxy difluorophosphinoxide,
Microwave spectra and molecular conformation of methoxy difluorophosphinoxide, 273
Methyl fluoroformate,
The structure of methyl fluoroformate from microwave spectroscopy and ab initio calculations, 471
Molecular motion,
Optimal design of external fields for controlling molecular motion: application to rotation, 425
Multi-body correlations,
Local symmetry, multi-body correlations and the cancellation effect, 253
Muscarinic agonists,
The hydrogen-atom environment of the ether oxygen atom in crystal structures of some representative muscarinic agonists, 287
Mutually bonded particles,
On the geometrical arrangements of mutually bonded particles of quantum systems, 93

Neutron powder diffraction,
Structure and valence from complementary anomalous X-ray and neutron powder diffraction, 383

Polyatomic molecules,
Calculation of the vib-rotational state density of polyatomic molecules by adiabatic switching, 157
$PPN^+HFe_3(CO)_{11}^-$,
EPR spectra of $FE_3(CO)_{11}^-$ ions and $[Fe_3(CO)_{11}^-]_2$ triplet ion-pairs trapped in single crystals of $PPN^+HFe_3(CO)_{11}^-$, 115
Propyl fluoride,
Microwave spectrum of iso-propyl fluoride and structure of iso-propyl halides, 207

Quantum systems,
On the geometrical arrangements of mutually bonded particles of quantum systems, 93

Ring puckering potential energy surface,
A two-dimensional ring puckering potential energy surface for ethylene carbonate from ab initio and flexible model computations, 325

Self-consistent field X_α scattered-wave method,
Corrections of overlapping spheres in the self-consistent field X scattered-wave method, 123

Triatomic molecules,
Triatomic molecules: meeting places for experiment and theory, 345
1,4,4-Trifluorocyclobutene,
Spectroscopy of 1,4,4-trifluorocyclobutene, 45
Trifluoromethyl mercaptan, CF_3,
Microwave spectrum, internal rotation, structure and dipole moment of trifluoromethyl mercaptan, CF_3SH, 185
Trifluoromethylgermane,
Microwave spectrum and structure of trifluoromethylgermane, 457